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Dear SCALE Sponsors:

Fiscal Year 2015 Report on SCALE Maintenance and Development

Enclosed is a report summarizing SCALE code system maintenance and development activities for fiscal year 2015. The attached report includes a table summarizing the sponsors and funding for SCALE maintenance and development activities. Given the wide range of activities covered, we recognize that some of you may desire additional information on one or more specific subjects. Please contact us if you have questions or would like more information on any subject.

Sincerely,

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SCALE Maintenance and Development for Fiscal Year 2015

I. Introduction

SCALE is a widely used suite of tools, including nuclear data, for nuclear systems modeling and simulation that provides comprehensive, verified and validated, user-friendly capabilities for criticality safety, reactor physics, spent fuel and radioactive source term characterization, radiation shielding, and sensitivity and uncertainty analysis. SCALE is developed and maintained within the Reactor and Nuclear Systems Division of the Oak Ridge National Laboratory (ORNL). For more than 30 years, regulators, licensees, and research institutions around the world have used SCALE for nuclear safety analysis and design. SCALE provides a "plug-and-play" framework that includes three deterministic and three Monte Carlo radiation transport solvers that are user-selected based on the type of problem being solved. Hybrid deterministic/Monte Carlo methods are also included to optimize solution performance and expand the realm of problems that can be accurately solved using Monte Carlo methods. SCALE includes the latest nuclear data libraries for continuous-energy and multigroup radiation transport as well as activation, depletion, and decay calculations. SCALE's graphical user interfaces assist with accurate system modeling, visualization, and convenient access to desired results.

This report summarizes the maintenance and development activities performed for the SCALE code system during fiscal year 2015. The primary goal of the SCALE maintenance activities is to ensure that the SCALE code system continues to meet the needs of sponsors and users by providing verified and validated results and remaining current with state-of-the-art computing technology. Ongoing maintenance activities ensure reliability by identifying and correcting discrepancies, providing enhancements to current capabilities, and programming for portability to different computing platforms. A thorough software configuration management process is used in performing these activities to assure adequate testing, documentation, and software control. Development activities involve major enhancements to existing modules as well as development of new modules, data libraries, and user interfaces. These activities employ current computing and programming techniques. The current public version of SCALE is 6.1, which was released in July 2011. The fifth beta release of SCALE 6.2 was provided to select early testers through 2015, with final release of SCALE 6.2 planned in FY16.

The maintenance and development of SCALE are sponsored by several organizations as shown in Table 1. Sponsors supporting ongoing maintenance activities are listed in the top portion of Table 1, while specific feature development activities are listed in the bottom portion of the table. The U.S. Nuclear Regulatory Commission (NRC) has been the historical lead sponsor in the development of SCALE, with support provided by both the Office of Nuclear Material Safety and Safeguards (NMSS) and the Office of Nuclear Regulatory Research (RES) since 1976. SCALE maintenance and development activities have been co-sponsored since 1987 by the Department of Energy (DOE) and the National Nuclear Security Administration (NNSA).

This report consists of five additional sections. Section II provides an overview of the current release of SCALE. Section III describes the major SCALE maintenance activities. Section IV summarizes the FY15 SCALE development activities for the projects listed in Table 1. Section V summarizes the new capabilities that are being developed for the next major release, SCALE 6.2.

Table 1. SCALE Sponsors and Funding for Fiscal Years 2014–2016

Sponsor[a]	Project Description	FY 2014 Funding ($K)	FY 2015 Funding ($K)	FY 2016 Funding Estimate ($K)
SCALE Maintenance Tasks				
DOE/NE/NFST	SCALE Maintenance and User Support	100	100	0
DOE/NNSA/NCSP	SCALE Maintenance & User Support [b]	695	720	1100
DOE/PCP	SCALE Maintenance	0	100	100
NRC/NMSS/SFST	SCALE Maintenance & Modernization	590	500	500
NRC/RES	SCALE Maintenance for Lattice Physics	185	185	185
Maintenance Subtotal		**1570**	**1605**	**1885**
SCALE Development Tasks				
A. DOE/NE/NEAMS	ORIGEN Integration	200	250	230
B. DOE/NE/NFST	UNF Characterization Enhancements for SCALE	250	0	0
C. NRC/RES	SCALE Lattice Physics Acceleration with Simplified Input	585	707	104
D. NRC/RES	SCALE Interface for SNAP	452	100	0
E. NRC/RES	Automated Characterization of Spent Fuel Pools	45	131	0
F. NRC/RES	Lattice Physics Code Performance Assessment	55	300	200
G. NRC/RES	SCALE/TRITON Acceleration	0	89	0
H. NRC/RES	Shift – Integration of SCALE Nuclear Stochastic Methods	0	150	150
I. NRC/RES	AMPX Modernization for SCALE Nuclear Data Libraries	0	200	150
J. CAS/SINAP	SCALE Enhancements for FHR	0	151	500
Development Subtotal		**1587**	**2078**	**1334**
GRAND TOTAL		**3157**	**3683**	**3219**

[a] Acronyms:

CAS = Chinese Academy of Sciences
FHR = Fluoride Salt-Cooled High-Temperature Reactor
NCSP = Nuclear Criticality Safety Program;
NE = Office of Nuclear Energy;
NEAMS = Nuclear Energy Advanced Modeling and Simulation;
NFST = Nuclear Fuels Storage and Transportation Planning Project
NMSS = Office of Nuclear Material Safety and Safeguards;
NNSA = National Nuclear Safety Administration;
PCP = Packaging Certification Program;
RES = Office of Nuclear Regulatory Research;
SFST = Spent Fuel Storage and Transportation;
SINAP = Shanghai Institute of Nuclear and Applied Physics;
UNF = Used Nuclear Fuel.

[b] Support only for criticality safety portion of SCALE.

II. Current Release of SCALE

SCALE 6.1 was released on July 22, 2011, providing several new features such as enhanced lattice physics capabilities and multigroup Monte Carlo depletion, improved options and capabilities for sensitivity and uncertainty analysis calculations, improved flexibility in shielding and criticality accident alarm system calculations with automated variance reduction, and new options for the definition of group structures for depletion calculations. The release of SCALE 6.1 required the coordination of 40 staff members under a quality assurance framework for development, testing, documentation, and deployment. The SCALE 6.1 development team focused on improved robustness via substantial additional regression testing and verification for new and existing features. The improved focus on the quality process has provided dividends in terms of improved efficiency for maintenance and development, and improved reliability for the sponsors and the users of SCALE. For example, 10 updates were issued for SCALE 6.0 over its 2.5-year life cycle to provide patches for issues that were identified after release. In contrast, only two technical patches have been issued during the three years since the release of SCALE 6.1, with no technical updates issued since February 2013.

The SCALE code system continues to provide capabilities for the analysis needs of the multi-agency programs that support SCALE. Additionally, the system continues to grow in popularity with domestic and international users with over 3971 licenses issued for SCALE 6.1 through September 2015, as shown in Fig. 1. Of the 3971 licenses, over 2718 were issued to new users who had not previously licensed any version of SCALE. At the end of FY14, there are over 6700 individuals in 55 nations licensed for one or more versions of SCALE, as represented by the map of nations with licensed SCALE users shown in Fig. 2.

The distribution of SCALE to end-users is subject to U.S. export control regulations, and each user must be individually licensed through an authorized distribution center. SCALE licenses are primarily issued through the Radiation Safety Information Computational Center (RSICC) at ORNL with mirrors at the Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA) Data Bank in France and the Research Organization for Information Science and Technology (RIST) in Japan. Any license fees collected for the distribution of SCALE are retained by these organizations to offset the costs of background checks and media duplication, and no part of the license revenue is used to support SCALE activities. RSICC’s current license recovery fee is $150 or $650 per user, depending on the level of export control review required. The fee is waived for all requests from U.S. universities. Through support of the NCSP, the fee is waived for users who are directly supported by the NCSP or users who are performing nuclear criticality safety work with SCALE.

Training courses and workshops on SCALE 6.1 continue to be popular with end users. Training is provided by developers and expert users from the SCALE team. Courses provide a review of theory, description of capabilities and limitations of the software, and hands-on experience running problems of varying levels of complexity. In FY15 a total of 14 weeklong courses were presented at ORNL, the OECD/NEA Data Bank, U.S. NRC headquarters, and user facilities. Additionally, two conference workshops were presented at topical meetings. In total, SCALE training was presented to 196 participants from 22 nations. The training courses are funded through user registration fees and are self-sustaining.

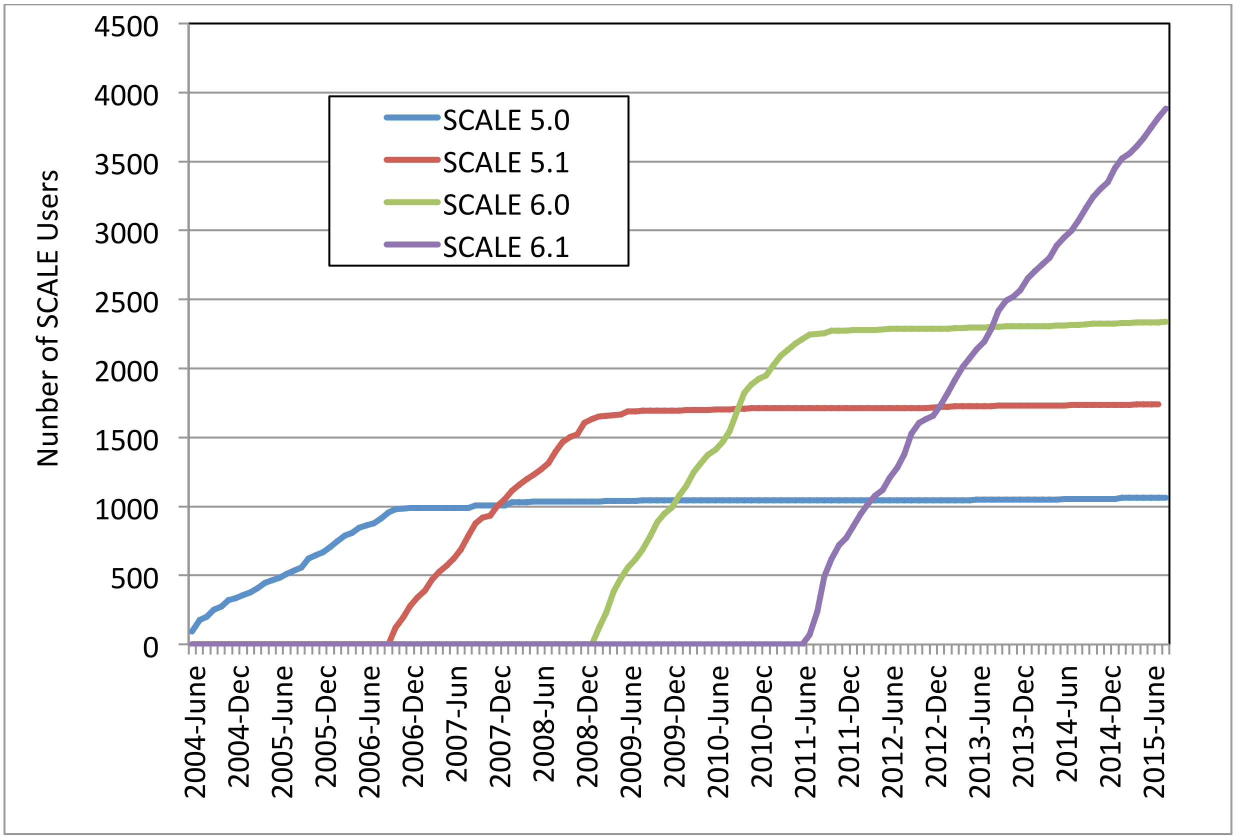

Fig. 1. Number of SCALE licenses issued for SCALE 5.0–6.1.

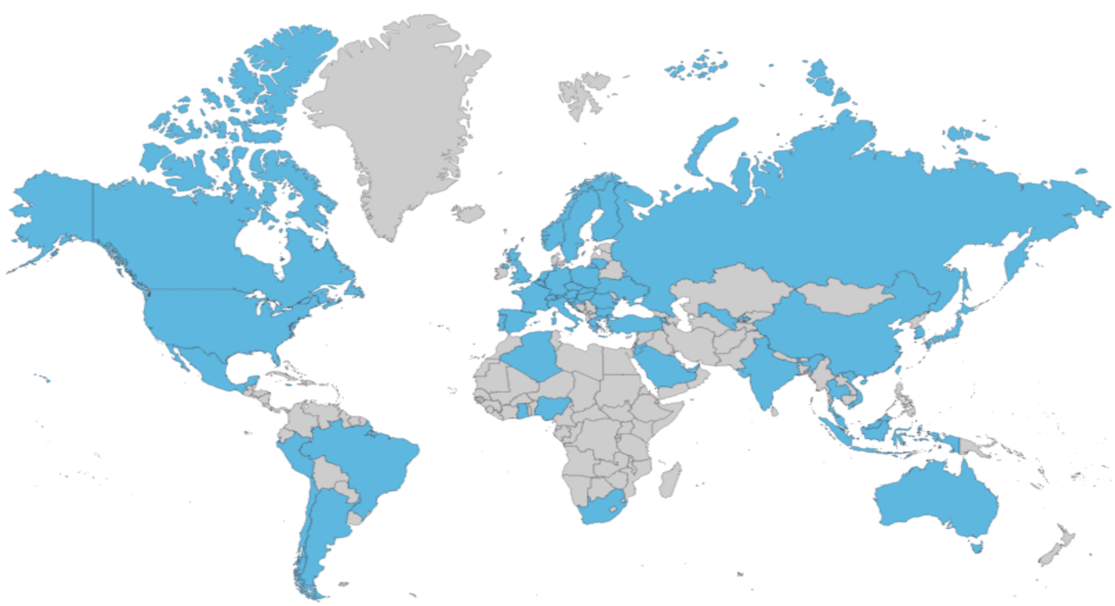

Fig. 2. Nations with Licensed SCALE Users.

III. SCALE Maintenance and Development Activities

SCALE maintenance activities provide an essential foundation for all activities related to reliable development and use of SCALE. Maintenance activities include quality assurance, development coordination, build and test infrastructure, and support for all existing capabilities and features. Recently, the SCALE team has focused efforts on infrastructure modernization by reviewing and incrementally updating components and procedures, which had evolved over a 30-year period, with modern software development practices and quality assurance standards. An essential component of this ongoing activity is the development of a modern framework for SCALE analysis, which enables rapid development of advanced methods, parallel operation, and easy integration of SCALE tools with other analysis packages. Each of the activities shown in Fig. 3 are described in more detail below.

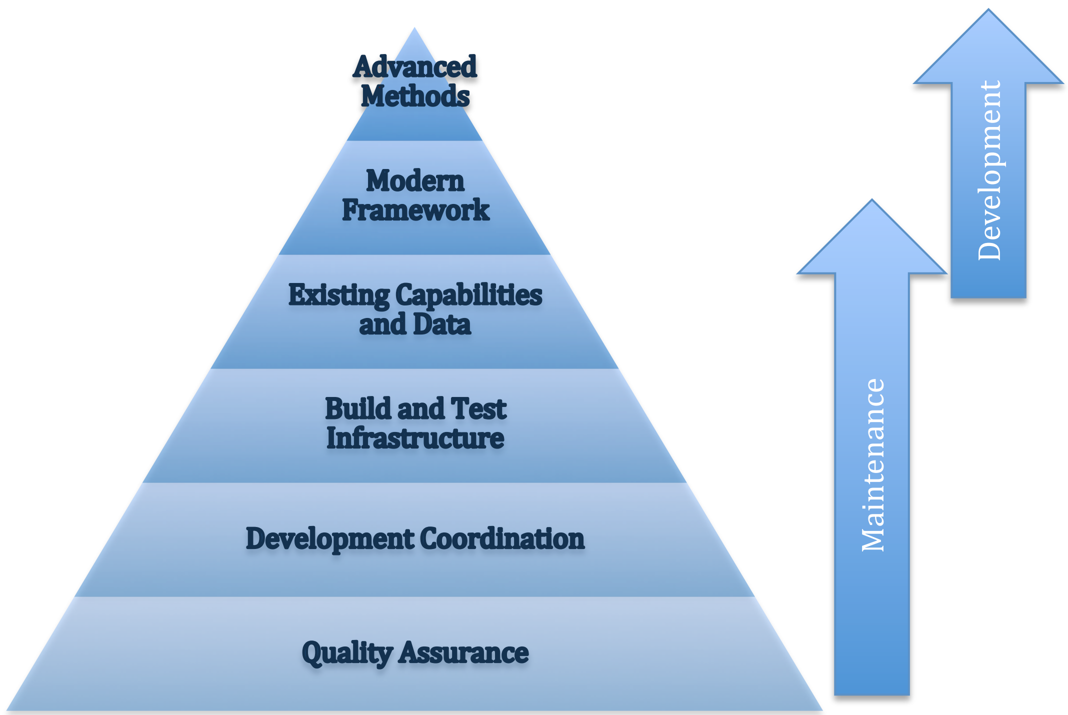

Fig. 3. SCALE Activities Diagram

III.A. Quality Assurance

Activities classified as maintenance begin with the establishment of the quality assurance (QA) framework that is applied to all SCALE codes and data. The SCALE QA program is kept current with international consensus standards (ISO-9001-2008, ASME NQA-1), U.S. Department of Energy orders (DOE 414.1D), NRC guidelines (NUREG/BR-0167) and the ORNL Standards-Based Management System. A review of the SCALE QA plan is performed annually by the ORNL Reactor and Nuclear Systems Division (RNSD) Software QA Board. The SCALE QA plan continues to be viewed as a model plan both inside and outside ORNL. It was the topic of several meetings with other software development teams domestically and internationally in FY15.

III.B. Development Coordination

The activities of SCALE staff members are coordinated to facilitate consistency throughout the project, especially in the application of quality assurance, development practices, and testing strategies. The SCALE team structure is shown below in Fig. 4.

The SCALE Leadership Team consists of the SCALE Manager, line managers, program managers, and developers as designated by the SCALE Manager. The Leadership Team meets regularly to discuss the current status and make programmatic and managerial decisions regarding SCALE. New roles of Deputy Manager, filled by Matt Jessee, and Software Development Coordinator, filled by Rob Lefebvre, were established in FY15 to better align program management and development activities throughout the project.

SCALE development teams are organized to coordinate work activities within given technical areas. Each team meets independently to plan and coordinate work activities. The teams are organized such that members from different work areas are included on multiple teams to improve communication and coordination between work areas. Although the activities of most teams are supported by targeted development tasks, coordination of the teams and review of their work is supported as a maintenance activity.

A weekly forum for developers and users is conducted to maintain a productive dialog and collaborative mission among developers, users, and managers within ORNL.

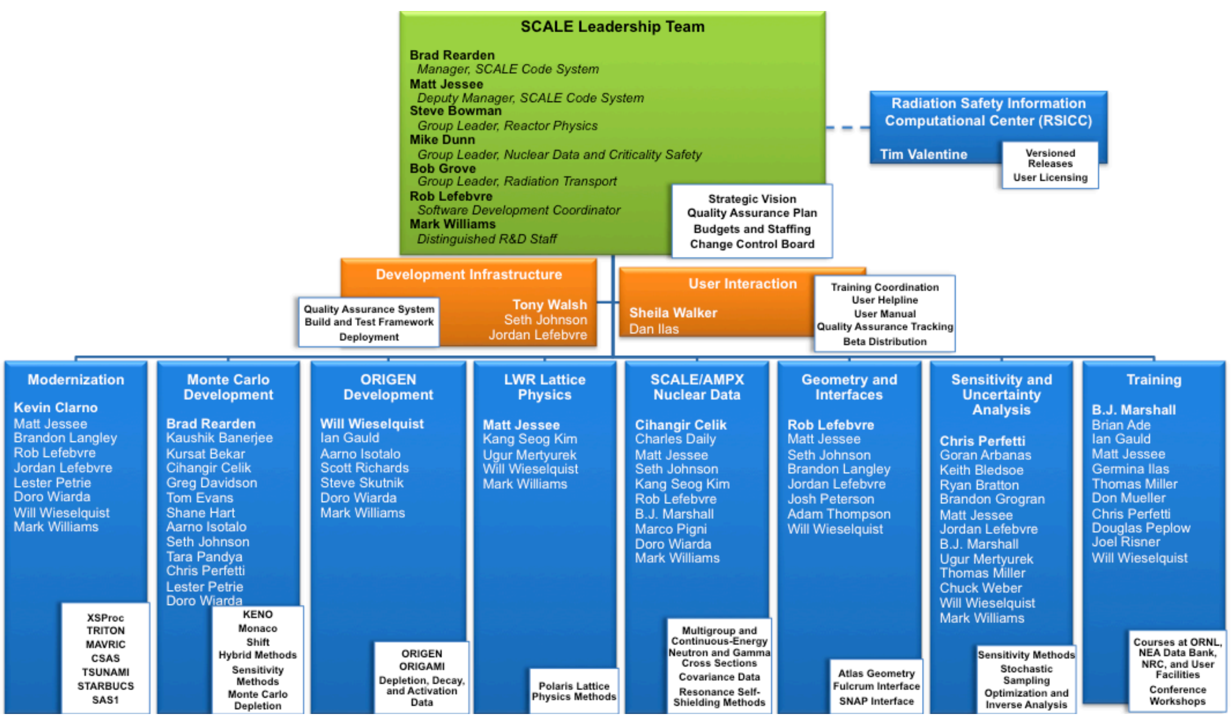

Fig. 4. SCALE Team Structure

III.C. Build and Test System

The foundation of any ongoing software project is the ability to routinely compile and test the software and data and provide continual support for the latest hardware and compilers. For SCALE, this foundation is provided as a maintenance activity.

After each incremental update to the source code, a suite of over 2000 test cases is run on each of dozens of computer platform configurations, including Linux, Mac, and Windows with different compilers and compiler options. This rigorous testing is performed dozens of times each day, resulting in the quantification of performance with approximately 150,000 tests per day. The results of the tests and the associated changes are reported to an internal website, known as the SCALE Dashboard. All developers can review the Dashboard to monitor the performance of numerous SCALE features on different platforms with different compilers using a pass/fail metric without the need to configure and run all of these tests themselves. In FY15, the number of systems continually building and testing SCALE was increased to obtain even finer quantification of the impact of individual changes. The hardware shown in Table 2, which consists of 288 processors and 872 GB RAM, is dedicated to running automated SCALE testing, 24 hours a day, 7 days a week.

Table 2. SCALE Continuous Integration Hardware

Platform	Hardware
Linux	• 8 cluster nodes each with 8 processors and 32 GB RAM • 1 dedicated computer with 64 cores and 256 GB RAM
Mac	• 3 Mac Pro computers each with 16 processors and 20 GB RAM • 2 Mac Pro computers each with 24 processors and 64 GB RAM
Windows	• 2 Windows 7 computers each with 8 processors and 16 GB RAM • 1 Windows 7 computer with 16 processors and 12 GB RAM • 1 Windows 2012 Server with 32 processors and 128 GB RAM

All changes to SCALE source code are recorded and versioned in a repository system. This system streamlines the development process, facilitate easier collaboration between developers, and provide easier quantification of changes to improve the QA review process.

III.D. Existing Capabilities and Data

SCALE 6.2 consists of approximately 2,000,000 lines of source code for 77 executable modules, 43 GB of nuclear data in approximately 9,000 files, and more than 4,000 pages of user documentation. With the previously mentioned 6700 licensed users of SCALE 5.0–6.1 in 55 nations, extensive communication is required. The SCALE team provided ongoing support to users by addressing approximately 709 inquiries during FY15 through scalehelp@ornl.gov e-mail. Additionally, an online discussion forum is available for SCALE users to post and review issues as a community (https://groups.google.com/forum/#!forum/scale-users-group). User communication in the form of website postings and newsletters is also provided.

Targeted development tasks generate dozens of new capabilities each year, and at the end of each development task, enhancements and user support for these features, additional testing and bug fixes, and integration of new features with existing features are supported as maintenance activities.

III.E. Modern Framework

In the SCALE 6.1 framework, a calculation involves a subset of the 89 independent computational modules, each executing in serial through progressive sequences where data are passed between modules through the computationally expensive process of reading and writing to the hard disk through file input/output (I/O). The vision set forth in the SCALE Modernization Plan calls for a modern framework where the majority of data transfers occurs in-memory and many of SCALE's computational components will be able operate on parallel computers from multi-core desktop machines to Linux clusters to the fastest supercomputers. The development of components within the modern SCALE framework is supported as ongoing maintenance of existing features. Where the update of a particular component is required, the best practices of modern software development are employed to provide for minimal development and maintenance costs in the future. The majority of FY15 SCALE maintenance support from all sponsors was focused on a modernization effort to realize substantial gains for SCALE 6.2.

The foundation of modern SCALE is a modular C++ software framework for efficient operation that also enables parallel computations. Individual computational components communicate through an efficient in-memory Application Programming Interface (API) instead of slow file I/O to the hard disk. Another advantage in the use of APIs for communication between components is that they allow for clear requirements on the data input and output of each modular component. Each capability that provides an API is referred to as a Module. Where internal tests are applied to ensure that data passed through the API meet all requirements of the Module, linkages with other Modules can be efficiently modified without disrupting any part of the overall system. The concept of individual functional modules as standalone executable programs will diminish as individual physics capabilities are consolidated into a unified executable program capable of performing all SCALE functionality within an efficient parallel infrastructure. Additionally, the modern API-based framework enables the development of a modern graphical user interface (GUI) that implements the same Modules used for computational analysis, removing the need to develop and maintain a feature twice, once for computational use and again for the GUI.

Examples of foundational modular capabilities that evolved to production-level status in FY15, with continuing enhancements expected in FY16, include:

- XSProc for multigroup cross section resonance self-shielding, energy group collapse, and spatial homogenization
- Continuous-energy and multigroup physics for Monte Carlo analysis
- ORIGEN depletion, decay and activation analysis and associated utilities
- Geometry package for Monte Carlo and Method-of-Characteristics (MoC) transport and visualization

Even though most SCALE modules have many of the same needs, such as reading the input file, reading cross-section data, and printing output, most of these functionalities have been independently implemented in each legacy code. Thus, a simple update such as modifying the format of a binary data library would require modification of dozens of SCALE modules that access the same data. A key component of modernization is the introduction of SCALE Resources that provide a single API for each of these common functionalities. To reduce the burden on individual computational modules related to reading and writing these custom-formatted files, the Resource class provides functionality related to disk access and file format in a centralized, testable location. Any SCALE module that needs Resource data simply requests the data, which are returned in memory from the Resource to the Module.

With the use of Resources, any new features in a data format can be updated in a single location (i.e., the Resource) and be immediately provided to all modules that benefit from the new data. Other modules that use the same Resource but do not require the new data can continue to operate as before with no impact from the change to the Resource. Many SCALE Resources provide a loader interface that enables the same data to be stored in multiple formats, which may be desired by different projects. The data format may be updated and translated based on the particular project needs across various hardware platforms.

Examples of SCALE Resources include, but are not limited to:

- Multigroup cross-section data libraries
- SCALE Standard Composition Library
- Continuous-energy cross-section data libraries
- Cross-section covariance libraries
- Activation, depletion, and decay data libraries
- Isotopic composition data

Input processing in SCALE has traditionally been split across each of the modules and the SCALE driver, where each module individually parsed a text input file, resolved interdependencies within this input stream, and processed these data for use in the calculation. This system of input processing presents possibilities for errors or development delays and can provide an inconsistent user experience, as similar features in different sequences can be implemented differently. To mitigate these difficulties, the new SCALE Parser has been created. The consistency and completeness of the input file is confirmed as the input is read and individual input blocks are provided through an API to the modules that use them. Once fully implemented across all SCALE Modules, the Parser will facilitate enhancements to input formats to provide convenience and consistency throughout SCALE.

A substantial FY15 modernization initiative and priority for SCALE 6.2 was the implementation of a modernized SCALE sequence framework that allows for the use of the modernized XSProc module for multigroup resonance self-shielding. XSProc utilizes the modern components described above and implements capabilities for problem-dependent temperature interpolation, calculation of Dancoff factors, resonance self-shielding using Bondarenko factors with full-range intermediate resonance treatment, as well as use of continuous-energy resonance self-shielding in the resolved resonance region. Cross sections can be provided as microscopic data for each nuclide or macroscopic data for each material in the original group structure. Additionally, a flux-weighting spectrum can be applied to collapse to a coarser group structure and/or to integrate over volumes for homogenized cross sections. The flux-weighting spectrum can be input by the user or calculated using one-dimensional coupled neutron/gamma transport. XSProc integrates and enhances the capabilities previously implemented independently in BONAMI, CENTRM, PMC, WORKER, ICE, and XSDRNPM, with some additional capabilities that were provided by MIPLIB and SCALELIB. The use of the modern XSProc sequence instead of individual legacy codes of previous versions of SCALE generally results in the preparation of cross sections in about 1/3 the time.

For SCALE 6.2, nearly all sequences will operate from the modern framework using XSProc. Many improvements in historical SCALE computational biases for multigroup calculations are realized with algorithm enhancements implemented in XSProc during modernization combined with enhancements in the multigroup data itself. In particular, the historical 400-500 pcm bias for LWR calculations is reduced to a much more acceptable value of 100 pcm. Unfortunately, the need to focus on methodology improvements to mitigate historical biases reduced the resources that could be allocated towards the realization of parallel computing capabilities for XSProc in SCALE 6.2. However, parallel Monte Carlo calculations with KENO, which were completed prior to FY15, are available in SCALE 6.2 with sequences that use KENO (i.e. CSAS, TSUNAMI, TRITON); parallel used fuel characterization calculations can be performed with ORIGAMI Automator; and parallel uncertainty quantification can be performed with Sampler. After the finalization of SCALE 6.2, work will resume to follow the modernization plan and realize parallel capabilities for resonance self-shielding with XSProc, parallel depletion with ORIGEN, as well as many other opportunities for performance enhancements.

A new consolidated user interface for SCALE, called Fulcrum, is being finalized for initial deployment with SCALE 6.2 to provide for input editing, model visualization, job execution, and data visualization. Fulcrum implements modern components such as the Parser for input generation; data Resources for standard compositions, nuclear data and computed results; and modern geometry for model visualization. Fulcrum is written in C++ and will be available on all supported platforms (Linux, Mac, and Windows). When completed, possibly across several SCALE releases, Fulcrum will replace the previous GUIs GeeWiz, OrigenArp, KENO3D, Javapeño, PlotOpus, MeshView, ChartPlot, and ExSITE.

III.F. Advanced Methods

The development of advanced methods in SCALE is generally not provided for as a maintenance activity. Advanced methods are developed as targeted tasks unless an incremental advancement is required to correct a discrepancy or enhance an existing feature for compatibility with a new feature. However, once an advanced method is completed, there are often QA and maintenance activities required to continue to provide support for it. Thus, as new features are integrated into SCALE, the amount of maintenance required is incrementally increased, pending removal of deprecated features. Many recent and ongoing methods advancements are described in the next section.

IV. SCALE Major Development Activities in FY15 and Ongoing Activities for FY16

The following items summarize FY15 SCALE development activities for the projects listed in Table 1, where capabilities were specifically requested by the sponsoring organization.

IV.A. ORIGEN Integration (DOE/NE/NEAMS)

ORIGEN depletion capabilities are being updated to enable high-performance parallel computing. In FY15, the new ORIGEN modules LibraryBuilder, TransitionMatrixUpdater, and MultiZoneDepleter were updated and tested in depletion applications. The LibraryBuilder is responsible for constructing ORIGEN libraries given a set of nuclides and reactions desired for the current calculation. The TransitionMatrixUpdater enables the coupling of depletion and transport calculations, performs operations such as the group collapse of multigroup cross sections and interpolation of fission yields over each depletion step. The MultiZoneDepleter was integrated with the NEAMS reactor analysis product line, developed at Argonne National Laboratory, to enable massively parallel calculations. To ensure full operability and QA for these new capabilities, the LibraryBuilder and TransitionMatrixUpdater codes have replaced the functions performed in the COUPLE module, which performed similar functions in SCALE 6.1 and earlier versions, but was not suitable for use in the modern SCALE framework for parallel computing.

Continuing work in this area in FY16 is expected to focus on verification and validation, generation of simplified isotope libraries to accelerate calculations for specific reactor types, as well as continued improvement to the interfaces through user feedback.

IV.B. UNF Characterization Enhancements for SCALE (DOE/NE/NFST)

SCALE is used extensively within the NFST analysis tool UNF-ST&DARDS (Used Nuclear Fuels Storage, Transportation, and Disposal Analysis Resource and Data System). The TRITON lattice physics sequence of SCALE is used to generate libraries of burnup-dependent nuclear data for each individual type of UNF assembly. These libraries are subsequently used to quantify discharge nuclide concentrations of individual assemblies with the ORIGAMI sequence for use in cask-specific criticality safety analyses with KENO, shielding analyses with MAVRIC, and thermal analyses with COBRA-SFS, which is not part of SCALE. Features integrated through this task provide unique capabilities for used fuel analysis, such as direct import of isotopics as well as gamma emission spectral data from depletion and decay calculations to facilitate shielding analysis. Additionally, the Sourcerer tool was developed for burnup credit criticality safety analysis for used fuel transportation and storage packages with challenging fission source distributions that cannot be satisfactorily converged using conventional Monte Carlo techniques. In FY15, the features provided in beta releases of SCALE 6.2 were integrated with UNF-ST&DARDS to ensure interoperability, but no new activities to support used fuel analysis under this project are planned for FY16.

IV.C. SCALE Lattice Physics Acceleration with Simplified Input (NRC/RES)

The objective of this task is to develop a new faster two-dimensional (2D) light water reactor (LWR) lattice physics sequence within SCALE to efficiently generate assembly-specific few-group nuclear data libraries using hundreds of branch cases for use in diffusion-theory three-dimensional (3D) reactor core simulators. Another objective in the development of this new LWR-specific sequence was to implement simplified user input that is at least 10 times shorter than the current SCALE general geometry input in the TRITON code sequence. Additionally, it was desirable to easily model heterogeneous 2D lattices with features such as internal moderator regions and burnable absorbers without the traditional SCALE complexities of providing explicit Dancoff factors for use in resonance self-shielding calculations. The Polaris sequence utilizes a multigroup self-shielding method called the Embedded Self-Shielding Method (ESSM) and a new 2D MoC transport solver. The MoC solver was implemented and tested in FY12. The focus of FY13 development was on the implementation of the ESSM, the development of a new 56-group nuclear data library, the integration of the ORIGEN depletion solver, and the development of the simplified input format. Work in FY14 focused on the completion of the branch capability and resolution of calculational biases observed in preliminary versions. In FY15, Polaris was extended to support boiling water reactor (BWR) analysis. As the capabilities of Polaris mature, it will supplant TRITON for lattice physics analysis of common LWR fuels. However, TRITON will continue to serve analysis needs such as research reactors and new fuel or reactor designs.

IV.D. SCALE Interface for SNAP (NRC/RES)

The U.S. NRC supports a graphical user interface called SNAP (Symbolic Nuclear Analysis Package) to function as a standard graphical user interface for the agency's analytical codes. SNAP has been developed by Applied Programming Technology, Inc. (APT) to help the analyst avoid having to learn many different code input formats and modeling peculiarities. SNAP provides a standardized, portable and extensible GUI as well as visualization and code execution framework that currently facilitates the use of many NRC developed analytical codes with the plug-ins PARCS, TRACE, RELAP5, MELCOR, CONTAIN 2.0, COBRA-IE, and FRAP. The SNAP developers previously produced a preliminary plug-in for the TRITON sequence of SCALE based on features documented in SCALE 6.1.

Through this task, an interface to all input requirements of SCALE has been implemented to continually provide SNAP developers a means of supporting the most recent capabilities, including nuances of input such as allowed data ranges and interdependencies of parameters. Additionally, a new input validation capability has been created that checks SCALE input for completeness and reports discrepancies to the user prior to beginning a calculation. As capabilities are developed for integration with SNAP, SCALE maintenance support is leveraged to integrate these new tools into the Fulcrum user interface for deployment with SCALE, providing powerful capabilities for all SCALE users such as spell checking and input validation, auto-completion, and resolution of input values for interdependent variables. Preliminary activities in FY14 focused on the development of a format for communicating information from SCALE to SNAP. In FY15 the implementation of SCALE input definitions (aka “schemas”) for all SCALE sequences and the validation engine for checking SCALE input files were provided to the SNAP developers. Continuing efforts in FY16 will focus on providing simplified access to output results for display within the SNAP interface.

IV.E. Automated Characterization of Spent Fuel Pools (NRC/RES)

One application area for the ORIGEN code is to quantify source terms for spent fuel pool decay heat analyses as well as for reactor severe accident analysis with MELCOR. Quantification of the entire fuel inventory of a nuclear power plant (NPP) requires a large number of ORIGEN calculations as well as a significant amount of bookkeeping of quantities such as each assembly's enrichment, operating history, spent fuel pool residence times, and as-built heavy metal mass. Recent source term analysis for the Vogtle NPP required the creation of input files for over 2800 fuel assemblies with data consolidated from a variety of sources.

In this task, ORNL developed a simple GUI to perform the pre- and post-processing tasks for this type of analysis, implementing the new ORIGAMI code to more effectively quantify spent fuel source terms. The new ORIGAMI Automator takes assembly and operating data as input and executes the appropriate ORIGAMI cases to simulate the depletion and decay of all assemblies to generate binary concentrations files for each assembly with concentrations available at all specified time points in its life. The user can group assemblies by location (e.g. “unit1” or “pool1”) as well as user-defined groups that could be defined explicitly or in terms of grouping parameters like discharge date ranges or burnup ranges. The post-processing utility automatically creates plot files for the time-dependent responses in each defined group and stores the ORIGEN data in a MELCOR-compatible data file.

The ORIGAMI Automator interface within Fulcrum provides an intuitive means of creating input, executing calculations, and visualizing results. Initial activities in FY14 focused on software design included “wireframing,” or sketching the desired interface layout and defining internal data structures. Activities in FY15 realized the rapid implementation and demonstration of the capability.

IV.F. Lattice Physics Code Performance Assessment (NRC/RES)

The purpose of this task is to complete a performance assessment of SCALE lattice physics codes (TRITON and Polaris) for LWR calculations and publish the results in a NUREG/CR report. This report will serve as a reference document for NRC staff and SCALE users. This task also includes the use of continuous-energy KENO for reference calculations, leveraging previously developed models from the SCALE/VALID criticality safety benchmark suite as well as existing TRITON and Polaris models, where applicable. The test suite will cover a wide range of operating conditions and assembly designs used in past and current commercial PWRs and BWRs.

A list of benchmark calculations has been developed covering the LWR application space for UO_2 and MOX fuel. Critical benchmark experiments, primarily from the International Handbook of Evaluated Criticality Safety Benchmark Experiments (ICSBEP) and the International Reactor Physics Experiments (IRPhE) will be applied to assess the quality of nuclear data for lattice physics calculations. Validation of the Polaris and TRITON depletion calculations will be performed using available radiochemical assay (RCA) measurements. Additionally, TRITON and Polaris calculations will be benchmarked using applicable MOX and UOX fuel international numerical benchmarks for neutronic parameters and depletion calculations. Other numerical benchmarks to be employed include DOE Consortium for Advanced Simulation of LWRs (CASL) depletion verification for pin cell calculations and a PWR assembly test matrix for fuel assembly calculations. The effort is being coordinated with the PARCS development team at University of Michigan to ensure consistency across the NRC's modeling and simulation tools, and in particular to ensure that the appropriate parameters for NRC needs are being assessed.

In FY15 many calculations and comparisons were performed, leading to numerous improvements in methodologies, especially in appropriately applying recent enhancements in resonance self-shielding capabilities and nuclear data to produce more accurate results for both Polaris and TRITON as compared to reference continuous-energy Monte Carlo depletion results.

IV.G. SCALE/TRITON Acceleration (NRC/RES)

This task supports the overall SCALE modernization effort with a focus on the TRITON sequences for release with SCALE 6.2. This task supports the modernization of TRITON, especially with the integration of the XSProc module into modernized TRITON sequences for multigroup analysis. The already completed modernization of ORIGEN provides an opportunity to extend these efforts and implement modern ORIGEN interfaces into the updated TRITON sequences. This task, to be completed in early FY16, will integrate modern ORIGEN into TRITON sequences for 1D, 2D and 3D depletion analyses for release with SCALE 6.2.

IV.H. Shift – Integration of SCALE Nuclear Stochastic Methods (NRC/RES)

SCALE currently contains three legacy Monte Carlo codes: KENO-V.a and KENO-VI for criticality safety analysis (with limited depletion capabilities in TRITON) and Monaco for fixed-source neutron-gamma shielding analysis. The KENO codes can utilize SCALE multigroup or continuous-energy neutron cross sections. Monaco utilizes coupled neutron-gamma multigroup or continuous-energy cross sections. Each of these Monte Carlo capabilities was developed as an individual package to meet sponsor needs with unique features, and all are currently in production use. However, all SCALE Monte Carlo capabilities are built on the legacy framework of KENO, which dates back to the 1960s. This framework creates challenges for integrating new features, upgrading the codes for parallel operation, or performing rigorous unit testing to quantify the performance of each component inside the code.

Under recent internal ORNL Laboratory Directed Research and Development (LDRD) projects, a new modern parallel Monte Carlo code called Shift has been developed within a broader radiation transport infrastructure at ORNL. The outcome of these efforts is a robust parallel Monte Carlo framework that provides an unprecedented opportunity to implement SCALE Monte Carlo calculations on cutting edge hardware, ranging from desktop PCs to Linux clusters to supercomputers. The modular design of Shift makes it possible, in future development, to provide a variety of geometry and physics packages for users to create their models and perform analysis, all within the single Shift package.

The objective of the task is twofold: (1) integrate the massively parallel Monte Carlo code Shift into standard SCALE sequences; and (2) verify and validate Shift for application to reactor analysis and criticality safety problems through this front-end interface. The resulting Monte Carlo capability will enable users to perform high fidelity, continuous-energy Monte Carlo simulations for analysis of steady-state core neutronics, fuel burnup, and criticality safety applications. This effort was initiated in FY15 and will continue through FY18 where capabilities will be phased in during each year.

IV.I. AMPX Modernization for SCALE Nuclear Data Libraries (NRC/RES)

AMPX is the cross-section processing software package used to provide nuclear data libraries for the SCALE code system. AMPX plays a vital role because it provides an independent capability to generate continuous energy and multigroup cross-section data and cross-section covariance data for SCALE. Because the accuracy of SCALE calculations are dependent on the accuracy of the underlying nuclear data files, there is a strong need for reliable and accurate nuclear data processing capabilities to ensure confidence and reliability in nuclear analyses performed with SCALE (e.g., reactor physics, criticality safety, shielding, etc.). Recently, the SCALE and AMPX development activities were merged under the same QA system developed for SCALE, and AMPX codes are being deployed with SCALE 6.2, the first public deployment of AMPX since 1977. This task will see the modernization of several essential and cross cutting data resources, data formats, and nuclear data processing codes for continuous-energy and multigroup cross section and cross-section covariance data generation. This effort was initiated in FY15 and will continue through FY18 where capabilities will be phased in during each year.

IV.J. SCALE Enhancements for Fluoride Salt-Cooled High Temperature Reactor (CAS/SINAP)

Through a new Cooperative Research and Development Agreement that began in FY15, SCALE will be enhanced to provide continuous-energy and multigroup criticality safety, shielding and depletion capabilities to support the design and licensing of FHR systems in China. Some planned activities include incorporation of the double-heterogeneity multigroup resonance self-shielding capabilities into XSProc and the development of accurate, convenient, and efficient modeling of explicit double-heterogeneity geometry for continuous-energy Monte Carlo calculations.

V. Future Development

The SCALE team is dedicated to providing advanced features in the SCALE 6.2 release in FY16 and future releases. The team works to assure and improve reliability through use of modern verification techniques and ongoing validation. The nuclear data generated by the ORNL AMPX code system for all SCALE continuous-energy, multigroup, activation/decay, and covariance libraries will continue to be improved through an iterative development cycle that includes increased testing. Modernization plans for SCALE and AMPX include increased synchronization of development activities and shared resources between these two projects.

It is desirable to position SCALE for the future with an extensive reprogramming of existing capabilities to improve run-time performance and solution fidelity. The most significant changes planned for the future will be the ability to execute SCALE in parallel on multiple CPUs – whether on desktops, workstation clusters, or high-performance supercomputers. This strategy includes the development of a new Monte Carlo code capable of excellent parallel scaling on leadership class computing architectures, such as ORNL's TITAN machine with approximately 300,000 processors. Shift will leverage many SCALE modernization capabilities such as the input Parser, nuclear data Resources, and Modules for continuous-energy and multigroup physics, modular geometry, and ORIGEN. The staged migration and testing of individual SCALE capabilities in the modern framework ensures robust development, testing, and deployment. The long-term modernization plan includes full modularity and parallelization in SCALE 7.